

Magn. Reson. Discuss., referee comment RC2
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Comment on mr-2021-48

Oscar Millet (Referee)

Referee comment on "Virtual decoupling to break the simplification versus resolution trade-off in nuclear magnetic resonance of complex metabolic mixtures" by Cyril Charlier et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2021-48-RC2>, 2021

This contribution describes, in a very elegant way, the limitations of the HSQC experiment decoupling in metabolomics and offers a solution based on a dual spectra acquisition followed by decoupling during the processing time. The enclosed results show improved resolution in the peak multiplicities. The manuscript also includes a historical overview of the HSQC experiment, which is most appropriate since the paper is a special issue to honour Prof. Bodenhausen. I believe that the presentation is excellent, as it is the quality of the contribution and the potential scientific impact warrants its publication in MR. I only have a couple of minor suggestions for the author's consideration:

i) HSQC is not usually quantitative but I wonder if, with this approach, the peak volume information could also be included in the metabolomics analyses of complex mixtures. Perhaps it could be discussed in the text.

ii) Selective cross-polarization could also be used to alleviate multiplet complexity. Obviously this is at the expense of dimensionality but if the main goal of the experiment is the chemical shift assignment, it could be eventually useful. Moreover, Prof. Bodenhausen has been very active in developing such methodology.